Possible superconductivity in hetero-polar interfaces of CuCl/Si superlattices: (001) and (111)

S. H. RHIM, R. SANIZ, A.J. FREEMAN, Northwestern U., J.J. YU, Seoul Natl. U. — To investigate possible interfacial superconductivity in CuCl/Si superlattices, we carried out first-principles calculations using the highly precise FLAPW method. Two possible growth directions, (001) and (111), are compared through their band structures, density of states (DOS), charge densities and Fermi surfaces. While the (111) superlattice is always metallic, the (001) superlattice is metallic or insulating depending on the number of Si and CuCl layers. Both directions exhibit two dimensional (2D) character at the interfaces which is a result of charge transfer between CuCl and Si layers. For metallic superlattices, the 2D conduction bands at the interfaces, resemble the 2D Cu-O $dp\sigma$ bands of cuprate superconductors. To obtain $T_C$ based on conventional electron-phonon (e-p) interactions, we calculated the e-p coupling constant, $\lambda$, within the rigid muffin-tin approximation. The results indicate that while e-p coupling is present in both directions, it gives $T_C = 0.41 \sim 1.69$ K, i.e. one order of magnitude lower than the previously reported high transition temperature - which, if confirmed, would indicate a possible role for excitonic effects.

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